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ON A PATH FOLLOWING METHOD FOR SYSTEMS OF EQUATIONS.(U)
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C. B. Garcia* and T. Y. Li**

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ABSTRACT

We consider the set of points $y \in R^{n+1}$ satisfying $H(y) = 0$, where $H : R^{n+1} \to R^n$ is C^2 and 0 is a regular value. This set is a C^1 one-dimensional manifold and each component can be described by a curve $y(p)$. We describe a general predictor-corrector method for following $y(p)$. This method is shown to be convergent.

AMS (MOS) Subject Classifications - 90C99, 65H10

Key Words - Homotopy, path-following, systems of equations, continuation methods

Work Unit Numbers 2 and 5 - Other Mathematical Methods, Mathematical Programming and Operations Research

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SIGNIFICANCE AND EXPLANATION

~~Consider~~ the problem of finding one or all solutions to systems of equations, equilibrium, fixed points, or to dynamical systems is considered. In the last few years, a new method has emerged for solving this problem. The idea is to start at a given solution of a simpler problem and to follow a path of solutions as the path parameter (and hence, the problem) is gradually changed. This path is proved to exist via topological approaches and is shown to lead to the "right" place.

In this paper, ~~we describe~~ a general predictor-corrector method is described for following the curve. It is a globalization of the classical Davidenko approach. ~~We show~~ It is shown that the method can follow the path to any desired degree of accuracy and is convergent.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

ON A PATH FOLLOWING METHOD FOR SYSTEMS OF EQUATIONS

C. B. Garcia* and T. Y. Li**

§1. INTRODUCTION

In the last few years, a number of methods [1, 3, 6-9, 12, 15-17] have been suggested for following a curve $y(p)$, $p^0 \leq p \leq \bar{p}$ satisfying

$$H(y(p)) = 0$$

where $H : R^{n+1} \to R^n$ is a given twice continuously differentiable function. The map H is usually of a certain genre, e.g. the fixed point homotopy

$$H(y) \equiv H(x,t) = (1 - t)(x - x^0) + tF(x) = 0, \quad 0 \leq t \leq 1$$

or the Newton homotopy

$$H(y) \equiv H(x,t) = F(x) - (1 - t)F(x^0) = 0, \quad 0 \leq t \leq 1$$

where $x^0 \in R^n$ is some given starting point. Generally, however, H need not be a homotopy, but rather H could be a system which describes a state dynamically changing overtime [8].

These methods are globalizations of the Davidenko approach [2, 4, 5, 13, 21] for following a path $y(t) = (x(t),t)$ satisfying

$$H(x(t),t) = 0 .$$

The new methods differ from the Davidenko approach in that the path need not be parameterizable in the last variable t. In the new approaches, the paths are first proved to exist and lead to the "right" place whereas in the Davidenko approach the paths are simply assumed to exist and methods are described for following them.

In this paper, we describe a general predictor-corrector procedure for following a path. Such a procedure relates to methods as early as Lahaye [13] and Haselgrove [10].

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As special cases, we get the Euler predictor-corrector [1, 16, 17] and the elevator predictor-corrector [9]. In Section 3, we show that the procedure described converges.

§2. A PREDICTOR-CORRECTOR ALGORITHM

Given a C^2 map $H : R^{n+1} \to R^n$, we say its derivative satisfies a Lipschitz condition on R^{n+1} if there exists a $K > 0$ such that for all $z, y \in R^{n+1}$

$$\|H'(z) - H'(y)\| \leq K\|z - y\| \tag{2.1}$$

where H' is the Frechet derivative of H, $\|\cdot\|$ is the usual Euclidean norm and K is called the Lipschitz constant.

Let P be an open interval containing $[p^0, \bar{p}]$, for some sealars $p^0 < \bar{p}$ and let $y : P \to R^{n+1}$ be a smooth curve such that for $p \in P$, we have

(i) $\|\dot{y}(p)\| = 1$ for $p \in P$ (parametrized according to arc length) where $\dot{y}(\cdot) = \frac{d}{dp} y(\cdot)$

(ii) $H(y(p) = 0$ for $p \in P$ (2.2)

(iii) $H'(y(p))$ has rank n for $p \in P$, i.e., all points on the curve $y(P) \equiv \{y(p) | p \in P\}$ are regular.

Suppose our interest is to follow the curve $y(p)$, $p^0 \leq p \leq \bar{p}$. We design a <u>predictor-corrector</u> algorithm to follow this curve. It proceeds as follows. Let $y^0 \equiv y(p^0)$. First, the vector $\dot{y}^0$ is computed directly from the <u>basic differential equation</u> [7]

(i) $u_i = (-1)^i \det H'_{-i}(y)$, $i = 1, \ldots, n + 1$

(ii) $\dot{y} = \frac{u}{\|u\|}$ (2.3)

where H'_{-i} is H' with the ith column deleted. (We assume here that (2.3) yields the "correct orientation", in the sense that (2.3) evaluated at y^0 yields $\dot{y}^0$. Otherwise, the correct differential equation is

$$u_i = (-1)^{i+1} \det H'_{-i}(y), \quad i = 1, \ldots, n + 1$$

$$\dot{y} = \frac{u}{\|u\|}$$

is the correct differential equation).

Then we take any <u>unit</u> vector $b^0 \in R^{n+1}$ such that the cross product $b^0 \dot{y}^0 \geq \delta$ where $0 < \delta \leq 1$ is some tolerance value given apriori.

We calculate for $k = 0$ the vector z^k via

$$z^k = y^k + h\Delta p_k b^k \tag{2.4}$$

where h is some value $0 < h \leq 1$ given apriori, and $\Delta p_k > 0$ a value to be defined in the next section. z^0 is termed the <u>predictor</u>. Δp_k is the <u>maximum</u> step size that can be taken in the direction b^k. h is a parameter that controls the distance travelled along b^k. The smaller is the h, the "closer" will the curve be followed by the predictor-corrector method.

Next, we use the <u>Newton method</u> to come back to the curve. To accomplish this, define $G : R^{n+1} \to R^{n+1}$ by

$$\begin{aligned} G_i(z) &= H_i(z) \qquad i = 1,\ldots,n \\ G_{n+1}(z) &= b^k(z - z^k) \end{aligned} \tag{2.5}$$

where $b^k, z^k \in R^{n+1}$ are given. Setting $k = 0$ in (2.5), we calculate the Newton iterates, where $k = 0$ and $z^{0,0} \equiv z^0$,

$$z^{k,j+1} = z^{k,j} - G'(z^{k,j})^{-1} G(z^{k,j}) \qquad j = 0,1,\ldots, \tag{2.6}$$

The step described by (2.6) is called the <u>corrector</u> step. Each $z^{k,j}$ lies on the hyperplane $b^k(z - z^k) = 0$. This brings us to a point y^1 "farther along" on the curve.

Generically, suppose we are at $y^k \equiv y(p^k)$, $p^0 \leq p^k < \bar{p}$. We take b^k such that $b^k y^k \geq \delta$, $\|b^k\| = 1$. We calculate the predictor z^k of (2.4). Then, we compute the sequence $\{z^{k,j}\}$ from (2.6) where $z^{k,0} \equiv z^k$. This brings us to a point y^{k+1} "farther along" $y(P)$. We terminate the algorithm if y^{k+1} is sufficiently near $y(\bar{p})$. See Figure 2.1.

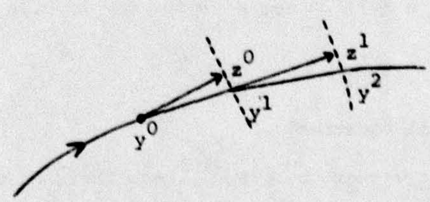

Figure 2.1

Given y^k, there are a number of ways that we can choose b^k. For example, we can choose $b^k = \dot{y}^k$. This is the Euler predictor. The resulting algorithm becomes the Euler predictor-corrector suggested in [15-17]. Then note that $b^k \dot{y}^k = 1$, so that the tolerance $\delta = 1$.

As another example, we can choose $b^k = (\operatorname{sgn} \dot{y}_i^k) e_i$ where e_i is the ith unit vector and where i is such that

$$(\dot{y}_i^k)^2 = \max_j (\dot{y}_j^k)^2 \tag{2.7}$$

The method is then the elevator predictor-corrector [9]. Note that $1 = \sum_j (\dot{y}_j^k)^2 \le (n+1)(\dot{y}_i^k)^2$ so that

$$b^k \dot{y}^k = |\dot{y}_i^k| \ge \frac{1}{\sqrt{n+1}} \tag{2.8}$$

so that $\delta = \frac{1}{\sqrt{n+1}}$. Further, note that if $b^k = (\operatorname{sgn} \dot{y}_i^k) e_i$, the Newton correctors (2.6) reduce to

$$\begin{aligned} z_{-i}^{k,j+1} &= z_{-i}^{k,j} - H'_{-i}(z^{k,j})^{-1} H(z^{k,j}) \\ z_i^{k,j+1} &= z_i^{k,j}, \qquad u = 0,1,\ldots, \end{aligned} \tag{2.9}$$

where $z = (z_{-i}, z_i)$.

In other words, the elevator predictor-corrector method is the classical Davidenko approach, except that there is an automatic change of coordinates when H'_{-i} is becoming singular. See Figure 2.2. (Indeed, this example shows that our convergence theory ought to handle also the important case where $\delta > 0$ is any small number.)

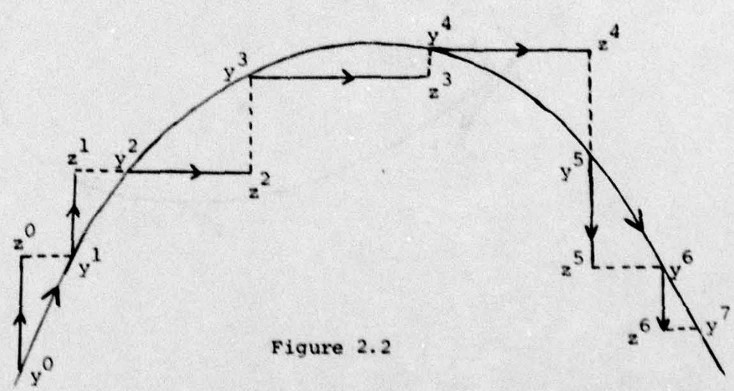

Figure 2.2

There are a number of problems that could arise relative to the predictor-corrector algorithm. For example, the hyperplane $b^k(z - z^k) = 0$ may not intersect the curve $y(P)$, whence (2.6) will not converge. This is the common problem encountered by a local Newton method or Davidenko method. Another conceivable problem is that the sequence $\{y^k\}$ generated might converge to a point $y^* \in y(P)$ far from $y(\bar{p})$, so that the method never reaches the end of the path. Finally, a serious problem that can occur is that y^{k+1} may be on the "wrong" portion of the curve. Then we could cycle indefinitely in a portion of the path. See Figure 2.3.

In the next section, we show that none of these problems can arise. There, we show that the predictor-corrector can be guaranteed to terminate with a point $y^n \equiv y(p^n)$ with $p^n \geq \bar{p} - \epsilon$, where $\epsilon > 0$ is some prescribed tolerance. To the best of our knowledge, these problems do not appear to have been thoroughly investigated in the literature. (See also the remark after Theorem 3.1).

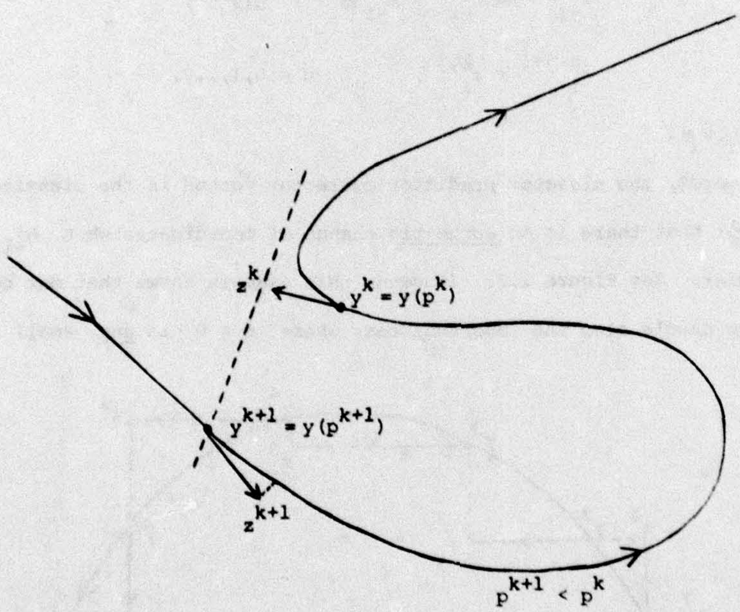

Figure 2.3

§3. CONVERGENCE OF THE PREDICTOR-CORRECTOR METHOD

In this section, we show the convergence of the predictor-corrector method. Throughout, we assume that H is C^2 and satisfies a Lipschitz condition (2.1). A curve $y(P)$ satisfying (2.2) is given.

The first theorem we show is

Theorem 3.1.

Consider $y^k \equiv y(p^k)$, $p^0 \le p^k \le \tilde{p}$. Then for any b^k such that $b^k\dot{y}^k \ne 0$, $\|b^k\| = 1$, there exists an open ball $N(y^k,\delta_1)$ with center y^k and radius δ_1 such that for any

$$z^k \equiv z^{k,0} \in N(y^k,\delta_1) \tag{3.1}$$

the Newton correctors (2.6) converge to a point $y^{k+1} \in y(P)$. Moreover, there exists a $\delta_2 > 0$ such that y^{k+1} is the unique solution of $G = 0$ in the open ball $N(z^k,\delta_2)$.

Proof: Consider $G'(z) = \begin{bmatrix} H'(z) \\ b^k \end{bmatrix}$

Since

$$\begin{bmatrix} H'(y^k) \\ b^k \end{bmatrix} \begin{bmatrix} H'(y^k)^t, \dot{y}^k \end{bmatrix} = \begin{bmatrix} H'(y^k)H'(y^k)^t & 0 \\ b^k H'(y^k)^t & b^k\dot{y}^k \end{bmatrix} \tag{3.2}$$

and since $[H'(y^k)^t, \dot{y}^k]$ and the right hand side matrix of (3.2) are nonsingular, $G'(y^k)$ is nonsingular. Hence, there is an open ball $N(y^k,\delta_3)$ of y^k with radius δ_3 and a $\gamma > 0$ such that

$$\|G'(z)^{-1}\| \le \gamma, \quad \text{for all } z \in N(y^k,\delta_3) \tag{3.3}$$

Next, by the continuity of G, for any $\varepsilon > 0$, there exists an open ball $N(y^k,\delta_1)$ such that

$$\|G(z)\| < \varepsilon \quad \text{for all } z \in N(y^k,\delta_1) \tag{3.4}$$

Lastly, note that if K is the Lipschitz constant for H',

$$\|G'(z) - G'(y)\| = \left\|\begin{matrix} H'(z) - H'(y) \\ 0 \end{matrix}\right\| \le K\|z-y\| \,. \tag{3.5}$$

Using (3.3)-(3.5), we can now show that for appropriate z^k, the hypotheses of the Newton-Kantorovich theorem [11, 18] holds. To see this, given δ_3, γ of (3.3) and K of (3.5), choose $0 < \delta_1 \leq \delta_3$ such that (3.4) holds for $\varepsilon = \frac{1}{2\gamma^2 K}$. Then, for $z^k \in N(y^k, \delta_1)$ we have

$$\alpha \equiv \|G'(z^k)^{-1}\| \; \|G'(z^k)\| K \leq \|G'(z^k)^{-1}\|^2 \|G(z^k)\| K < \gamma^2 \left(\frac{1}{2\gamma^2 K}\right) K = \frac{1}{2} .$$

Hence, the hypothesis of the Newton-Kantorovich theorem holds. Thus, the Newton iterates (2.6) coverage to a solution y^{k+1} of $G = 0$ which is unique in $N(z^k, \delta_2)$ where $\delta_2 \equiv (\gamma K)^{-1}[1 + (1 - z\alpha)^{1/2}]$.

This theorem closely relates to theorems proved in [16, 17]. However, note that the theorem above gives no information as to where on the curve y^{k+1} lies. For example, in Figure 2.3, y^{k+1} could be a point as near as we please to z^k, yet is such that $p^{k+1} < p^n$. To prevent such cases from occurring, we need a stronger result.

Consider $y^k \equiv y(p^k)$, $p^0 \leq p^k \leq \bar{p}$. Let b^k be such that $\|b^k\| = 1$, $b^k \dot{y}^k \neq 0$. Let

$$g(p) = b^k y(p) .$$

By the Implicit Function theorem, $\dot{g}(p) = b^k \dot{y}(p)$ is continuous in a neighborhood of y^k. There is an open ball $N(y^k, M_1)$ such that $y(P) \cap N(y^k, M_1)$ is a connected smooth path containing y^k and $\dot{g}(p) \neq 0$ for any $y(p) \in N(y^k, M_1)$.

<u>Proposition 3.2</u>.

For any $0 < M_2 \leq M_1$, there is an M_3, $0 < M_3 < M_2$ such that for any $z^k \in N(y^k, M_3)$

(i) $T(z^k) \equiv \{z \mid b^k(z - z^k) = 0\}$ intersects $y(P) \cap N(y^k, M_1)$ at a unique point, and

(ii) the point of intersection is in $N(y^k, M_2)$.

<u>Proof</u>: Let $H(z) = b^k z$ and let a_1, a_2 be such that $Q \equiv y(P) \cap N(y^k, M_2) = \{y(p) \mid a_1 < p < a_2\}$. Then, since g is strictly monotone in p for $y(p) \in N(y^k, M_1)$, $g(a_1) < g(p^k) = h(y^k) < g(a_2)$, or $g(a_1) > h(y^k) > g(a_2)$. There is an open ball

$N(y^k,M_3)$ such that $g(a_1) < h(z) < g(a_2)$ for all $z \in N(y^k,M_3)$ on $g(a_1) > h(z) > g(a_2)$ for all $z \in N(y^k,M_3)$.

Proposition 3.2.

For any $0 < M_2 \leq M_1$, there is an M_3, $0 < M_3 < M_2$ such that for any $z^k \in N(y^k,M_3)$

(i) $T(z^k) \equiv \{z | b^k(z - z^k) = 0\}$ intersects $y(P) \cap N(y^k,M_1)$ at a unique point, and

(ii) The point of intersection is in $N(y^k,M_2)$.

Proof: Let $H(z) = b^k z$ and let a_1,a_2 be such that $Q \equiv y(P) \cap N(y^k,M_2) = \{y(p) | a_1 < p < a_2\}$. Then, since g is strictly monotone in p for $y(p) \in N(y^k,M_1)$, $g(a_1) < g(p^k) = h(y^k) < g(a_2)$, or $g(a_1) > h(y^k) > g(a_2)$. There is an open ball $N(y^k,M_3)$ such that $g(a_1) < h(z) < g(a_2)$ for all $z \in N(y^k,M_3)$ or $g(a_1) > h(z) > g(a_2)$ for all $z \in N(y^k,M_3)$.

Suppose there exists a $z^k \in N(y^k,M_3)$ such that $T(z^k) \cap Q = \phi$. Then either $b^k(y(p) - z^k) > 0$ for all $a_1 < p < a_2$ or $b^k(y(p) - z^k) < 0$ for all $a_1 < p < a_2$. That is, $g(p) = b^k y(p) > h(z^k)$ for all $a_1 < p < a_2$ or $g(p) < h(z^k)$ for all $a_1 < p < a_2$. This is a contradiction, since g is continuous and $g(a_1) < h(z^k) < g(a_2)$. or $g(a_1) > h(z^k) > g(a_2)$. Hence, $T(z^k) \cap Q \neq \phi$, for all $z^k \in N(y^k,M_3)$.

Finally, $T(z^k) \cap y(P) \cap N(y^k,M_1)$ is a unique point since g is strictly monotone in p for $y(p) \in N(y^k,M_1)$.

The next proposition eliminates cases such as in Figure 2.3 from arising.

Proposition 3.3.

For $y^k \equiv y(p^k)$, $p^0 \leq p^k \leq \bar{p}$, let b^k be chosen such that $\|b^k\| = 1$, $b^k y^k > 0$. Then, if $0 < M_2 < \frac{1}{4} M_1$ and $0 < M_3 < \delta_1$ in proposition 3.2, where δ_1 is defined in (3.1), the Newton correctors (2.6) with starting point

$$z^k \equiv z^{k,0} = y^k + hM_3 b^k, \quad 0 < h \leq 1 \tag{3.6}$$

converges to a unique point $y^{k+1} \equiv y(p^{k+1})$ in $N(y^k,M_2)$. Moreover, we have $p^{k+1} > p^k$.

Proof: By proposition 3.2, there exists a unique $y(p^*) \in N(y^k,M_2)$ such that $b^k(y(p^*) - z^k) = 0$. We first note that

$$\|y(p^*) - z^k\| < 2M_2 . \tag{3.7}$$

Note that $y(p^*)$ is a solution of $G = 0$ defined by (2.5). Also, by Theorem 3.1, the Newton iterates converge to a point $y^{k+1} \equiv y(p^{k+1}) \in y(P)$.

Suppose $y^{k+1} \neq y(p^*)$. Then $y^{k+1} \notin N(y^k,M_1)$. Hence $\|y^{k+1} - z^k\| > M_1 - M_3 > 3M_2$ so that radius δ_2 of the ball $N(z^k,\delta_2)$ in Theorem 3.1 is greater than $3M_2$. From (3.7), this implies that $y(p^*) \in N(z^k,\delta_2)$, a contradiction of the uniqueness of solutions for $G = 0$ in $N(z^k,\delta_2)$.

Finally, we have $b^k(y^{k+1} - y^k) = b^k(y^{k+1} - z^k) + b^k(z^k - y^k) = b^k(z^k - y^k) = hM_3b^k\dot{b}^k > 0$. That is, for $g(p) \equiv b^k y(p)$, we have $g(p^{k+1}) > g(p^k)$. Since $\dot{g}(p) > 0$ for $y(p)$ in $N(y^k,M_1)$, $p^{k+1} > p^k$.

Let us reconsider the predictor-corrector method described in §2. Suppose we are at a point $y^k \equiv y(p^k)$, $p^0 \leq p^k < \bar{p}$ on the path. We choose b^k, $b^k\dot{y}^k \geq \delta > 0$, $\|b^k\| = 1$ where δ is some a priori given tolerance. (We must bound $b^k\dot{y}^k$ below by δ so as to avoid getting a sequence $\{b^k,y^k\}$ where $b^k\dot{y}^k \to 0$, which causes difficulties). By proposition 3.3, there is an M_3, $0 < M_3 < \delta_1$ such that if the predictor z^k is computed by (3.6), the Newton correctors (2.6) will come back to a point farther along the curve. Let $\Delta p_k \equiv \Delta p(y^k,b^k)$ of (2.4) denote the maximum number of such kind. By repeated use of the predictor-corrector method, we will generate a sequence $\{y^k\}$ on the curve $y(P)$. We terminate when we generate a point $y^n = y(p^n)$ such that $p^n \geq \bar{p} - \varepsilon$ for some prescribed tolerance $\varepsilon > 0$.

Theorem 3.4.

The predictor-corrector method terminates in a finite number of iterations.

In order to prove Theorem 3.4, we need the next lemma. Given $y^k \equiv y(p^k)$, $p^0 \leq p^k < \bar{p}$ and tolerance $\delta > 0$, define

$$q = \min\{\Delta p(y^k,b) \,|\, b\dot{y}^k \geq \delta/2,\ \|b\| = 1\} \tag{3.8}$$

where $\Delta p(y^k, b) < \delta_1$ is the maximum number such that for

$$z^k \equiv z^{k,0} = y^k + h\Delta p(y^k, b)b \tag{3.9}$$

the Newton correctors (2.6) (where b^k is replaced by b) will come back to a point farther along the path. Since the constraint set of (3.8) is compact, and since $\Delta p(y^k, b) > 0$ for all b satisfying the constraints of (3.8), we have

$$q > 0 . \tag{3.10}$$

<u>Lemma 3.5.</u>

There exists an open ball $N(y^k, M)$ of y^k such that for any $y \in N(y^k, M) \cap y(P)$, and any b such that $b\dot{y} \geq \delta$, $\|b\| = 1$, we have $\Delta p(y, b) > \frac{1}{2} q$.

<u>Proof</u>: Choose $0 < M < \frac{1}{4} q$, and M small enough such that for any $y \in N(y^k, M) \cap y(P)$, we have

$$b\dot{y} \geq \delta, \ \|b\| = 1 \ \text{ implies } \ b\dot{y}^k \geq \delta/2 . \tag{3.11}$$

Hence, by (3.8), $\Delta p(y^k, b) \geq q$. Moreover, for any $y \in N(y^k, M) \cap y(P)$, we have $N(y, \frac{1}{2}q) \subset N(y^k, q)$. Therefore, by (3.11), for any b such that $b\dot{y} \geq \delta$, $\|b\| = 1$ and any $z^k \in N(y, \frac{1}{2}q)$ we have $z^k \in N(y^k, q)$ so that Theorem 3.1 implies that the correctors (2.6) (where b^k is replaced by b) converge when started at z^k. Hence, $\Delta p(y, b) > \frac{1}{2} q$.

Finally, we may now prove Theorem 3.4.

<u>Proof of Theorem 3.4.</u>

Suppose the predictor corrector never ends. Then there is an infinite sequence $\{y^k\}$ such that $y^k \in y(P)$ for all k and $\lim_{k \to \infty} y^k = y^* \equiv y(p^*)$ for some $p^* \leq \bar{p} - \epsilon$.

But since $(y^{k+1} - z^k)(z^k - y^k) = 0$, we have

$$\|y^{k+1} - y^k\|^2 = \|y^{k+1} - z^k\|^2 + \|z^k - y^k\|^2 \geq \|z^k - y^k\|^2 = (h\Delta p_k)^2$$

Hence, $\lim_{k \to \infty} (y^{k+1} - y^k) = 0$ implies $\lim_{k \to \infty} \Delta p_k = 0$. This is a contradiction, since by lemma 3.5, for all y^k sufficiently near y^*, we have $\Delta p_k > \frac{1}{2} q$.

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We consider the set of points $y \in R^{n+1}$ satisfying $H(y) = 0$, where $H : R^{n+1} \to R^n$ is C^2 and 0 is a regular value. This set is a C^1 one-dimensional manifold and each component can be described by a curve $y(p)$. We describe a general predictor-corrector method for following $y(p)$. This method is shown to be convergent.

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